

On the Complexity of One-class SVM for Multiple Instance Learning

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Abstract

In traditional multiple instance learning (MIL), both positive and negative bags are required to learn a prediction function. However, a high human cost is needed to know the label of each bag—positive or negative. Only positive bags contain our focus (positive instances) while negative bags consist of noise or background (negative instances). So we do not expect to spend too much to label the negative bags. Contrary to our expectation, nearly all existing MIL methods require enough negative bags besides positive ones. In this paper we propose an algorithm called “Positive Multiple Instance” (PMI), which learns a classifier given only a set of positive bags. So the annotation of negative bags becomes unnecessary in our method. PMI is constructed based on the assumption that the unknown positive instances in positive bags be similar each other and constitute one compact cluster in feature space and the negative instances locate outside this cluster. The experimental results demonstrate that PMI achieves the performances close to or a little worse than those of the traditional MIL algorithms on benchmark and real data sets. However, the number of training bags in PMI is reduced significantly compared with traditional MIL algorithms.

Keywords: Multiple Instance Learning; One-class

1 Introduction

Multiple instance learning (MIL) is introduced by [9] to solve the drug activity prediction problem. During the past years, MIL approaches have been applied successfully to many real applications such as image categorization [5, 6, 19], image retrieval [24, 22], tracking [3], web mining [21], gene expression [15] and medical diagnosis [10]. In traditional supervised learning, each instance(feature vector) of training set corresponds to one given label. By contrast, every set of instances (not one instance) is associated with a given label in MIL. Each instance set is called a “bag”. If a bag contains at least one positive instance, it is labeled as positive and negative otherwise. It is unknown which instance is positive in each bag. In other words, only bag level label is available while instance level label is not in positive bags. The task of MIL is to learn a concept to predict the label of an unseen bag.

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In nearly all existing MIL algorithms, both positive and negative bags are required during the training phase. But only the positive instances are our focus generally and the negative instances are unrelated to our interest. For example, if we attempt to learn a concept of face, the face patches in an image are positive instances and other non-face images are labeled as negative bags. According to this preference, we are willing to concentrate on labeling face images and ignore non-face images as much as possible. Non-face images are not our interest. However, negative bags are not less and even much more than positive in many real data sets such as Corel [7]. The availability of negative bags requires a high cost. So labeling on negative bags brings great inconvenience in real applications. In addition, it takes more time to label one negative bag than positive in that every instance must be confirmed to be negative. In contrast, remaining instances in one positive bag can be ignored if only one positive instance is found. The labeling on negative bags increases label cost significantly. So it is necessary to design a method using only positive bags to learn.

One related work is [22]. His method is simply to solve a query problem, in which an extra positive instance must be provided by user. The most similar instance in every positive bag to this provided positive instance is considered positive. This solution has the following disadvantages. Firstly, the positive instance is difficult to provide or unavailable in some applications. So [22] can be applied to a limited range of settings. Secondly, some bags contain more than one positive instances. [22] cannot select multiple positive instances accurately in one bag. Thirdly, the performance of this algorithm depends mostly upon the positive instance given by user. It causes the prediction accuracy of [22] is too sensitive to the provided positive instance. In contrast, our proposed algorithm in this paper requires no additional positive instance in most cases. Therefore, our proposed algorithm can solve a wider range of problems.

In this paper, a new algorithm called PMI(Positive Multiple Instance) is proposed, which learns a concept from only positive training bags. PMI is designed based on the assumption that the positive instances constitute one compact cluster in feature space and most negative instances locate outside this cluster. PMI works with two major steps—training and query. The training step is to convert the problem of learning with only positive bags into a one-class classification problem [18] to get a classifier f . If the instance level label is not available, PMI terminates and outputs f as the concept. Otherwise, go to the query step. The query step is to select an instance to query its label from instances positively labeled by the classifier f in the previous training step. If the queried instance is negative, remove the instances positively labeled by the classifier f from the training bags and return to the training step. Otherwise, PMI outputs f as the desired concept and terminates. We provide the maximum number of queried instances theoretically. The queried instance number in real applications usually is far smaller than the theoretical result. The experimental results demonstrate that PMI achieves close performances to those of the traditional MIL algorithms on most data sets. Our contribution is that the training bags number can be reduced greatly at a little or no worse on accuracy. Negative bags are unnecessary for training in our method.

The remainder of this paper is organized as follows. We introduce PMI algorithm in Section 2 in detail. Section 3 illustrates PMI with experiments. We conclude on our work in Section 4 finally.

2 Our Proposed Algorithm

In this section, we propose PMI algorithm. One-class SVM [18] is involved in PMI, so a brief review on one-class SVM is presented here.

2.1 Review on One-Class SVM

The formal definition of one-class SVM is described as following. N d -dimensional instances x_1, x_2, \dots, x_N in feature space \mathbb{R}^d are given, where \mathbb{R} denotes real number field. The task is to learn a prediction function takes value +1 while capturing most given instances in a small region of feature space and -1 otherwise. One-class SVM maximizes the margin between the training instances and origin in feature space to obtain a decision hyperplane by the following formulation:

$$\begin{aligned} \min_{w, \rho, \xi, \nu} & \frac{1}{2} \|w\|^2 + \frac{1}{\nu N} \sum_i \xi_i - \rho \\ \text{s. t. } & (w \cdot \Phi(x_i)) \geq \rho - \xi_i, \\ & \xi_i \geq 0, w \in \mathbb{R}^d, \rho \in \mathbb{R}, \end{aligned} \quad (1)$$

where $\nu \in (0, 1)$ is a parameter to balance the regularization $\|w\|^2$ and the hinge loss $\sum_i \xi_i$, w and ρ are the weight coefficient and the bias in linear decision function respectively, ξ , $\xi^T = [\xi_1, \dots, \xi_n]$ denotes a slack variable vector, ξ_i is the i -th element of ξ , and $\Phi(x_i)$ is a nonlinear map function to x_i to deal with nonlinear boundary of training instances. A kernel function $ker(x, y)$ is defined to replace $\Phi(x) \cdot \Phi(y)$. Model 1 is a quadratic programming problem, which can be solved through its dual form:

$$\begin{aligned} \min_{\alpha} & \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j ker(x_i, x_j) \\ \text{s. t. } & 0 \leq \alpha_i \leq \frac{1}{\nu N}, \quad \sum_i \alpha_i = 1, \end{aligned} \quad (2)$$

where α_i is a Lagrange multiplying factor of x_i . The value of α_i is summarized into three categories according to where x_i locates:

1. $\alpha_i = 0 \rightarrow x_i$ locates inside positive instance region;
2. $\frac{1}{\nu N} > \alpha_i > 0 \rightarrow x_i$ lies on the prediction function boundary;
3. $\alpha_i = \frac{1}{\nu N} \rightarrow x_i$ falls outside the positive instance region.

The label of an unseen instance x is predicted by the following function:

$$f(x) = \text{sign}\left(\sum_i \alpha_i ker(x, x_i) - \rho\right), \quad (3)$$

where the function $\text{sign}(y)$ outputs +1 if $y \geq 0$ and -1 otherwise. If $f(x) \geq 0$, we assume that x should be similar to the training instances with a high likelihood. Otherwise, x is an outlier. ρ in Eq. (3) is computed:

$$\rho = \sum_i \alpha_i ker(x_i, x_j), \quad (4)$$

where x_j is a support vector, which implies that x_j locates on the boundary of decision function $f(x)$ and $f(x) = 0$.

Various complex separation hyperplanes can be described by different types of kernel functions, such as polynomial, RBF, sigmod or self-defined ones. RBF kernel is given by:

$$ker(x, y) = e^{\gamma \|x-y\|^2}, \quad (5)$$

where γ denotes a parameter to control how similar x is to y . In general, we assume that samples of interest locate inside closed regions in the feature space. RBF function is one of the most widely used kernel for its flexibility. We will use RBF as the default kernel function in the rest of this paper.

2.2 Our Proposed Algorithm

Our proposed algorithm PMI is introduced in detail in this subsection. At the beginning, we provide the formal definition of the problem PMI solves. A collection of bags $\{B_1, B_2, \dots, B_N\}$ are given as the training set. The i -th bag in the training set B_i contains N_i d -dimensional instances $B_i = [B_{i1}, \dots, B_{iN_i}] \in \mathbb{R}^{d \times N_i}$ and $B_{ij} \in \mathbb{R}^d$ is a d -dimensional instance, $j = 1, \dots, N_i$. We define an $d \times n$ matrix stacking all instances together $B = [B_1, \dots, B_N]$, where n denotes the total number of all instances in N bags. At least one positive instance resides in each bag of training set, but it is unknown which instance is positive. The same as the label rule in previous MIL approaches, a bag is positive if it contains at least one positive instance and is negative otherwise. Our goal is to learn a function to predict the label of an unseen bag. PMI works in two steps: training and query. If instance level label is available, PMI algorithm alternates between training and query step until the desired concept is obtained. Otherwise, PMI runs training step for once. The remainder describes the two steps explicitly.

2.2.1 Training Step

As is mentioned in Section Introduction, PMI assumes that positive instances be similar to each other in feature space. We explain this assumption in Figure 1. Take face identification as an example, the task is to learn a function to predict whether an image contains face or not. So the patches containing face are positive instances we are focus on in Figure 1 and the other non-face patches are negative instances. It can be easily found that face patches (red rectangles in Figure 1) look similar to each other while non-face patches are dissimilar. In summary, positive instances refer to one concept leading to the high similarity between positive and negative instances usually locate outside the region occupied by positive instances in feature space.

According to the previous explanation and illustration in Figure 1, we assume that most positive instances gather in a compact cluster and negative instances locate outside this cluster. At least one instance in most training bags resides in this positive cluster (the cluster composed of positive instances). Now we needs a function to describe the positive cluster. This function takes the value +1 in the positive cluster region and takes -1 elsewhere. We can apply this function on every instance in one bag to identify whether this bag is positive or not. But since we actually do not which instance is positive, the positive concept cannot directly be learned from positive instances.

As is stated in [2, 10], the selection of instances will be formulated as a combinatorial optimization problem, which is non-convex and difficult to solve especially when a global optimal solution

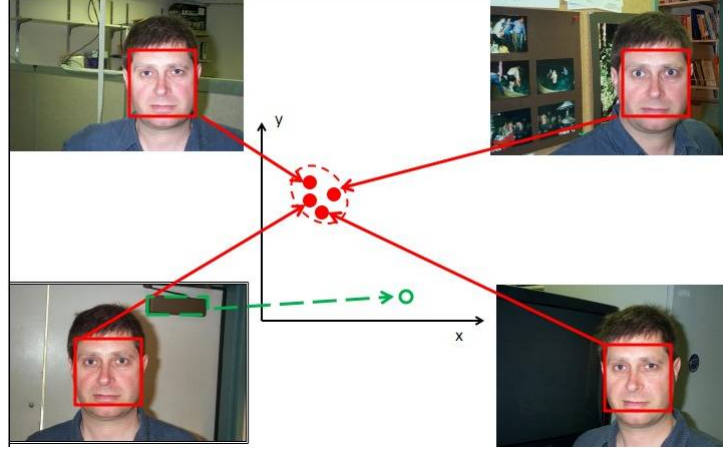


Fig. 1: It is illustrated positive instances are clustered in a small region and negative instances locate outside. The red solid points are positive and the green circle is negative.

is required. We tend to approximate one virtual instance b_i with a high likelihood to be positive for each training bag B_i . The desired concept can be learned from these approximated positive instances. To make our method efficient and easy to solve, a linear combination coefficient vector λ_i is used to convert each bag B_i to a virtual positive instance b_i in feature space:

$$\begin{aligned} b_i &= B_i \lambda_i = \sum_{j=1}^{N_i} B_{ij} \lambda_{ij}, \\ \text{s.t. } \sum_j \lambda_{ij} &= 1, \quad \lambda_{ij} \geq 0, \quad i = 1, \dots, N, \end{aligned} \tag{6}$$

where $\lambda_i = [\lambda_{i1}, \dots, \lambda_{iN_i}]^T$. Let λ denote the vector concatenating all λ_i , $\lambda = [\lambda_1; \lambda_2; \dots; \lambda_N]$. Assume that b_i is positive, b_i should be highly close to the positive instances in B_i . Furthermore, if B_{ij} is positive, λ_{ij} will be assigned a larger value and small otherwise. According to the assumption that the positive instances get similar to each other, all b_i should get close to each other in feature space. To keep the distances between b_i as small as possible, the variance between all b_i is minimized to obtain λ :

$$\begin{aligned} \min \quad & \sum_{i=1}^N (B_i \lambda_i - m_i)^T (B_i \lambda_i - m_i) \\ \text{s. t. } \quad & \sum_{j=1}^{N_i} \lambda_{ij} = 1, \quad \lambda_{ij} \geq 0, \end{aligned} \tag{7}$$

where $m_i = \frac{1}{N} \sum_{i=1}^N B_i \lambda_i$.

We define matrix Z_i with $n \times n$ size, $i = 1, \dots, N$. The diagonal elements in Z_i are 1 at location (j, j) , $j = N_{i-1} + 1, \dots, N_i$ in Z_i and 0 elsewhere. It satisfies that $\sum_{i=1}^N Z_i = I$, where I is an identity matrix with $n \times n$ size.

Eq. (7) is rewritten as a standard quadratic programming formulation:

$$\begin{aligned} \min \quad & \lambda^T \left(\sum_{i=1}^N [BZ_i - \frac{1}{N}B]^T [BZ_i - \frac{1}{N}B] \right) \lambda \\ \text{s. t.} \quad & \sum_{j=1}^{N_i} \lambda_{ij} = 1, \quad \lambda_{ij} \geq 0, \end{aligned} \quad (8)$$

where $[BZ_i - \frac{1}{N}B]^T [BZ_i - \frac{1}{N}B]$ is really symmetric and semi-positively definite, so $(\sum_{i=1}^N [BZ_i - \frac{1}{N}B]^T [BZ_i - \frac{1}{N}B])$ is also real symmetric and semi-positive definite. The non-zero part of $BZ_i \lambda$ is equal to $B_i \lambda_i$. The formulation Eq. (8) is a convex optimization problem.

To tackle nonlinear separable data, the kernel trick is applied to Eq. (8). We reformulate the $B^T B$ as the kernel matrix K , whose element K_{ij} at i -th row and j -th column is the kernel function value $\text{ker}(x_i, x_j)$, $i, j = 1, \dots, n$. Eq. (8) is reformulated:

$$\begin{aligned} \min \quad & \lambda^T \left(\sum_{i=1}^N [KZ_i - \frac{2}{N}KZ_i + \frac{1}{N^2}K] \right) \lambda \\ \text{s. t.} \quad & \sum_{j=1}^{N_i} \lambda_{ij} = 1, \quad \lambda_{ij} \geq 0. \end{aligned} \quad (9)$$

As λ is known by Eq. (9), we can learn the concept of positive instance from $\{b_i, \dots, b_N\}$ using one-class SVM method. The kernel function value between two virtual positive instances is computed:

$$\text{ker}(b_i, b_j) = \sum_{k=1}^{N_i} \sum_{r=1}^{N_j} \lambda_{ik} \lambda_{jr} \text{ker}(B_{ik} B_{jr}). \quad (10)$$

Eq. (2) is reformulated as the following:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j \sum_{k,r} \lambda_{ik} \lambda_{jr} \text{ker}(B_{ik}, B_{jr}) \\ \text{s. t.} \quad & 0 \leq \alpha_i \leq \frac{1}{\nu N}, \quad \sum_i \alpha_i = 1. \end{aligned} \quad (11)$$

As is described previously, α_i in three different ranges implies where b_i locates in feature space. According to the value of α_i , bag B_i can be summarized as two kinds:

Definition 1 (*Support Bag*) For a bag B_i , if $0 < \alpha_i < \frac{1}{\nu N}$, then B_i is a “**Support Bag**”.

Definition 2 (*Outlier Bag*) For a bag B_i , if $\alpha_i = \frac{1}{\nu N}$, then B_i is an “**Outlier Bag**”.

By solving Eq. (11), the prediction function is:

$$\begin{aligned} f(B_i) &= \text{sign} \left(\max_{r=1, \dots, N_i} l(B_{ir}) \right), \\ l(B_{ir}) &= \sum_{j=1}^N \alpha_j \sum_{k=1}^{N_i} \lambda_{jk} \text{ker}(B_{ir}, B_{jk}) - \rho, \end{aligned} \quad (12)$$

where B_i is the predicted bag. ρ is computed:

$$\rho = \sum_{i=1}^N \alpha_i \sum_{k=1}^{N_i} \sum_{r=1}^{N_j} \lambda_{ik} \lambda_{jr} \text{ker}(B_{ik}, B_{jr}), \quad (13)$$

$$B_j \text{ satisfies: } 0 < \alpha_j < \frac{1}{\nu N}.$$

If it holds that $\max_j f(B_{ij}) = f(b_i), \forall i = 1, \dots, N$, ν satisfies the following theorem:

Theorem 1 *If $\rho(\neq 0)$ is the solution of Eq. (11) and $\max_j f(B_{ij}) = f(b_i) (\forall i = 1, \dots, N)$, the following holds: ν is the upper bound on the fraction of outlier bags.*

Proof Each bag is converted to one virtual instance by Eq. (6). Theorem 1 is easy to be validated from *proposition 4* in [18][17]. \square

If $f(B_i) = f(b_i) = 1$, at least one instance in B_i must locate on or inside the prediction function boundary (Eq. (12)). However, $f(B_i) = f(b_i) = 1$ cannot be guaranteed completely. In other words, when the virtual instance $b_i = B_i \lambda_i$ falls inside or on the function boundary, all instances in B_i may fall outside. It can be expressed as follows:

$$f(b_i) = +1 \neq \max_{j=1, \dots, N_i} f(B_{ij}) = -1. \quad (14)$$

So the assumption $\max_j f(B_{ij}) = f(b_i)$ in Eq. (1) does not always hold in the proof of Theorem 1. It causes the upper bound on outlier bags fraction is larger than ν sometimes. To keep the upper bound of outlier bags fraction on ν , our solution is to select the instance B_{is_i} that is closest to function boundary in each bag B_i and add it to the training set. We learn a new prediction function with the updated training set. Now the training set consists of both the selected instances $\{B_{is_i}\}$ and the virtual instances $\{b_i\}$. The parameter to control the number of outlier bag becomes $\frac{\nu}{2}$ since the number of training instances is $2N$ here. B_{is_i} is determined by the following criterion:

$$s_i = \arg \max_{j=1, \dots, N_i} l(B_{ij}). \quad (15)$$

The new decision function will replace the result of Eq. (11) by solving the following quadratic programming problem:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{p,q} \alpha_p \alpha_q \sum_{p,q} \text{ker}(x_p, x_q) \\ \text{s. t.} \quad & 0 \leq \alpha_p \leq \frac{1}{\nu 2N}, \quad \sum_p \alpha_p = 1 \\ & x_p, x_q \in \{b_i\} \cup \{B_{is_i}\}, \\ & i = 1, \dots, N, \quad p, q = 1, \dots, 2N. \end{aligned} \quad (16)$$

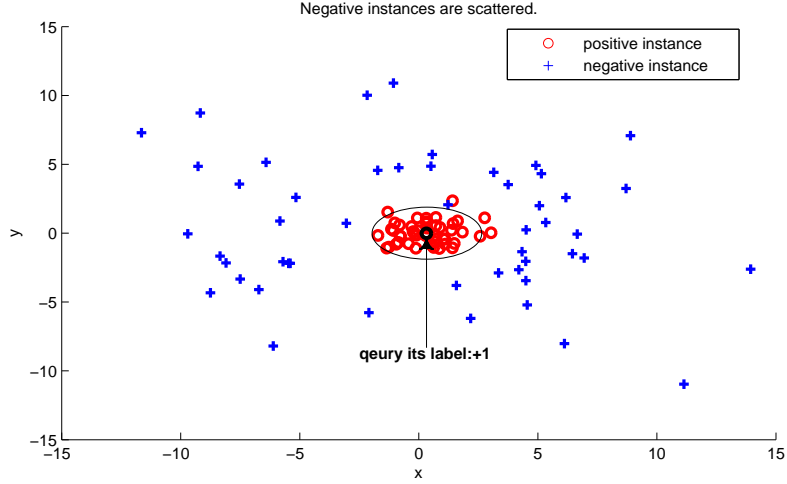


Fig. 2: The distribution of positive (red) and negative (blue) instances is illustrated. The positive instances are similar to each other and gathered compactly. By comparison, the negative are dissimilar and scattered.

The prediction function from Eq. (16) is:

$$\begin{aligned}
 f(B_i) &= \text{sign}\left(\max_{r=1,\dots,N_i} l(B_{ir})\right) \\
 l(B_{ir}) &= \sum_{p=1}^{2N} \alpha_p \text{ker}(B_{ir}, x_p) - \rho, \\
 \rho &= \sum_{p=1}^{2N} \alpha_p \text{ker}(x_p, x_q), \quad x_q \text{ satisfies: } 0 < \alpha_q < \frac{1}{\nu 2N}.
 \end{aligned} \tag{17}$$

Now Eq. (17) is the desired prediction function instead of Eq. (12) if $\exists i, f(B_i) \neq f(b_i)$.

In Eq. (16), the upper bound on outlier bags fraction satisfies the following theorem:

Theorem 2 *If $\rho(\neq 0)$ is the solution of Eq. (16), the following holds: ν is the upper bound on the fraction of outlier bags.*

Proof If b_i falls outside and B_{is_i} locates inside the prediction function boundary, it holds $\max_j f(B_{ij} = f(B_{is_i}) = 1)$. In the worst case, there are $\frac{\nu}{2} \times 2N = \nu N$ instances in the set $\{B_{is_i}\}$ falls outside the prediction function boundary. This implies that the largest number of outlier bags is νN . So in the worst case the upper bound on outlier bag fraction reaches ν in Eq. (17). \square

2.2.2 Query Step

As is described previously, the positive instances should gather compactly in feature space. On the other hand, the distribution of negative instances is unknown. If the negative instances are scattered and dissimilar to each other greatly (Figure 2), we can get the prediction function to enclose most positive instances in feature space easily. However, negative instances are also

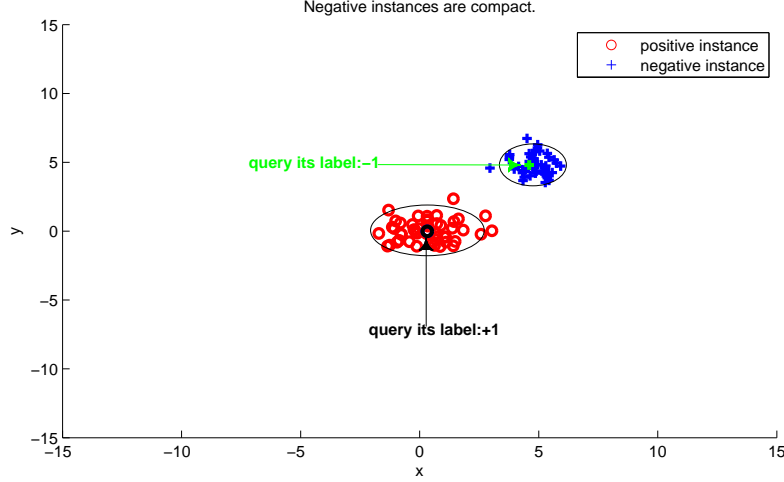


Fig. 3: The distribution of positive (red) and negative (blue) instances is illustrated. Both the positive and negative instances are clustered. The number of positive instances (red) is equal to that of negative, but negative occupy a smaller circle region. So the negative cluster looks more compact than positive. The query step is needed. The black elliptical circle is positive cluster’s boundary. The queried instances (black and green) locate closest to the centers of positive and negative cluster respectively.

clustered sometimes (Figure 3) and even share a higher similarity than positive. Take face identification as an example, some face images are used to learn a prediction function and each image contains the same background (for example, tree, sky and so on). If there is a higher similarity between background patches than face ones, the variance of negative instances get smaller than that of positive. The result of training step is to enclose the negative instances with a higher similarity instead of the desired positive cluster. To avoid this result, our method requires to confirm whether the cluster enclosed by prediction function boundary is composed of positive or negative instances. We select an instance B_{qr} characterizes this cluster best to query its label. The queried instance shares the same label with the most member of this cluster. If the queried instance is positive, this cluster is positive with a high likelihood and negative otherwise.

The function $l(x)$ is a good measure on the membership of x to the resulted cluster. When x locates outside the cluster, $l(x) < 0$ and $l(x) \geq 0$ otherwise. The larger $l(x)$ is, the closer x gets to the center of the cluster. So the instance B_{qr} with maximum $l(x)$ characterizes this cluster best and is selected to query its label:

$$\begin{aligned} B_{qr} = \arg \max_{i,j} l(B_{ij}) \\ \text{s.t.} \quad l(B_{ij}) \geq 0 \end{aligned} \quad (18)$$

If prediction function boundary is like a circle, the queried instance usually locates closest to the circle center than others (Figure 3). If B_{qr} is negative, this cluster should be also negative. Otherwise, this cluster should be positive. Figure 3 illustrates the queried instance location when there are more than one cluster in feature space.

If the queried instance is negative, we update the current training bags by removing the instances satisfying $\{B_{ij} | l(B_{ij}) \geq 0\}$ and go back to the training step for a second instance label query. PMI works in such a recycle between training and query steps. PMI terminates when the queried instance is positive or there is one empty bag in training set. PMI is summarized in Algorithm 1.

In Algorithm 1, the number of queried instances satisfies the following:

Theorem 3 *In Eq. (11), if the parameter $\nu < \frac{1}{N}$, the maximum number of queried instances is $\min_{i=1,\dots,N} N_i - 1$. Otherwise, the maximum number of queried instance is $\lceil \frac{n}{(1-\nu)N} \rceil - 1$.*

Proof According to Theorem 1, $\nu < \frac{1}{N}$ implies there is no outlier bag in the current training set. The step 4 in Algorithm 1 guarantees that there is at least one instance B_{ij} satisfying $f(B_{ij}) = 1$ for every bag B_i , $i = 1, \dots, N$. Thus, At least one instance in each bag must be removed in every instance removal operation. If one training bag gets empty after removal, PMI terminates at the step 6 in Algorithm 1. Therefore, the maximum number of queried instances is $\min_{i=1,\dots,N} N_i - 1$.

If $\nu \geq \frac{1}{N}$, at least $(1 - \nu)N$ instances will be removed at the step 8 according to Theorem 1. So the maximum number of queried instances is $\lceil \frac{n}{(1-\nu)N} \rceil - 1$, where $\lceil x \rceil$ denotes the minimum integer number not smaller than x . \square

The step 6 in Algorithm 1 needs some further explanations. If all members of one bag are labeled positive, these instances belongs to the positive class in that each training bag contains at least one positive instance.

However, the instance label information is not always available. When it is difficult to query instance label, our solution is to assume that the dissimilarities between negative instances are larger than positive ones. Thus, Algorithm 1 terminates at the step 4 and outputs the prediction function $f(x)$ without running the query step. In most real applications, negative instances cover a diverse range of backgrounds or noise. Therefore, it is almost impossible that negative instances share a higher similarity than positive. It is high likely to achieve the concept on positive instance after only one training step. The experimental results in the next section illustrate that our hypothesis is applicable for most of data sets. It also implies that the maximum query number in Theorem 3 is not a tight bound. The number of queried instance label usually is far smaller than the result in Theorem 3 and close to 1 mostly. It suggests that the cost of instance label query is very limited, which is much lower than that of labeling a large number of negative bags.

Algorithm 1 PMI

Input: the training bags $\mathcal{B} = \{B_i, i = 1, \dots, N\}$;

kernel function parameters;

ν ;

- 1: Solve Eq. (9) to get λ ;
- 2: Solve Eq. (11) to get a prediction function $f_0(\text{Eq. (12)})$. Set $f = f_0$;
- 3: If there exists one bag B_i satisfying both $\alpha_i < \frac{1}{\nu N}$ and $\max_{j \in 1, \dots, N_i} f(B_{ij}) = -1$, select an instance B_{is_i} by Eq. (18) from every training bag B_i , $i = 1, \dots, N$;
- 4: Solve Eq. (16) to get a prediction function $f_1(\text{Eq. (17)})$. Set $f = f_1$;
- 5: If no instance label information is available, PMI terminates;
- 6: If there is one bag B_i , $i = 1, \dots, N$ satisfying that $\forall j \in 1, \dots, N_i$ $f(B_{ij}) = 1$, PMI terminates;
- 7: Select the most certain instance by Eq. (18) to query its label;
- 8: If the queried label is positive, PMI ends. Otherwise, update the training set \mathcal{B} by removing the instances $\forall i, j$ B_{ij} satisfying $f(B_{ij}) = 1$. Go back to the step 1;

Output: prediction function f ;

2.3 Time Complexity Analysis

The time complexity analysis of PMI involves Eq. (9), Eq. (11), Eq. (16) and the number of the queried instances. These three objective functions Eq. (9), Eq. (11) and Eq. (16) are three quadratic programming problems with the time complexities $O(n^3)$, $O(N^3)$, $O(N^3)$ respectively. Since $n > N$ in general, the term $O(n^3)$ dominates the time complexity of PMI. According to Theorem 3, the number of queried instances is related to $\frac{n}{N}$. So the time complexity is $O(\frac{n^4}{N})$. But in real applications, the queried instance number is much smaller than the theoretical result in Theorem 3 and can be approximated to a constant. The time complexity of PMI is close to $O(n^3)$.

3 Experiments

This section presents the experimental results on five benchmark and one face image data sets. We evaluate PMI compared the traditional MIL algorithms. To solve the quadratic programming problem in Eq. (2), the optimization toolbox “Mosek” [16] is used.

3.1 Benchmark Data Sets

Five benchmark data sets are used in our experiment. They are Musk1, Musk2, Elephant, Fox and Tiger, which were used frequently to test new MIL algorithms in previous studies[9, 10, 2]. Both Musk1 and Musk2 come from UCI data set web site [20]. And the other three derive from Corel image set [7]. The details of five data sets are described in Table 1.

Table 1: five datasets details

data set	bag number (positive)	mean bag size	dimensionality
Musk1	92(47)	5.17	166
Musk2	102(36)	64.69	166
Elephant	200(100)	6.96	230
Fox	200(100)	6.90	230
Tiger	200(100)	6.10	230

The accuracies of PMI on five benchmark data sets are recorded in Table 3. To compare with PMI, we also provide the performances [10, 2] of several other traditional MIL algorithms. These traditional MIL algorithms are mi-SVM [2], MI-SVM[2], EM-DD[23] and MICA[10].

The same with previous MIL studies, 10-fold cross validation strategy is used to get the accuracies of PMI. Both positive and negative bags are divided into 10 folds randomly and one fold positive and negative bags are selected as testing set. The remaining 9 fold positive bags (without negative ones) are the training set. The difference between that of PMI and 10-fold cross validation used in traditional MIL studies is that the training set of PMI does not contain 9 fold negative bags.

Table 2: The numbers of positive bags used for training in PMI and other MIL algorithms are listed.

	Musk1	Musk2	Elephant	Fox	Tiger
PMI	47	36	100	100	100
mi-SVM	92	102	200	200	200
MI-SVM	92	102	200	200	200
MICA	92	102	200	200	200
EM-DD	92	102	200	200	200

Table 3: The classification accuracies of five algorithms on the five data sets are presented. The results are percentage of correctly predicted bags. These accuracies are average results of 10 runs.

	Musk1	Musk2	Elephant	Fox	Tiger
PMI	79.1 \pm 1.1	85.1 \pm 1.2	78.3 \pm 0.7	57.9 \pm 1.5	52.5 \pm 1.0
mi-SVM	87.4	83.6	80.0	57.9	78.9
MI-SVM	77.9	84.3	73.1	58.8	66.6
MICA	84.4	90.5	82.5	62.0	82.0
EM-DD	84.8	84.9	78.3	56.1	72.1

Table 2 shows the numbers of positive bags used for training in PMI and other traditional MIL algorithms. Table 3 reports the accuracies of five approaches on five benchmark data sets. These accuracies are the average of 10 runs. PMI terminates at the step 5 of Algorithm 1 and returns $f(x)$ due to no available instance label of these five data sets. PMI achieves close results to those of the other traditional MIL methods mostly. The result on Musk2 is better than mi-SVM, MI-SVM, EM-DD, but worse than MICA. Musk2 has only 39 positive bags, which are obviously smaller than the negative bag number 63. So it is exciting that PMI achieves the similar performance using much fewer training bags (only positive bags) to those of other MIL approaches. PMI achieves a little lower accuracy on Musk1 than mi-SVM, MICA and EM-DD, but a little larger than MI-SVM. The results of PMI are close to those of the other MIL methods on Elephant and Fox.

According to the performance comparison in Table 3, if the traditional MIL methods achieve a high accuracy on one data set, PMI can also obtain similar result. But when the performance of traditional MIL method becomes very low (only about 60% accuracy on Fox data set), PMI will get a worse result than those of traditional MIL methods. We explain the phenomenon as follows. If there is a enough large margin and no overlap between positive and negative instances, the traditional MIL methods with positive and negative training bags usually get a perfect accuracy. Due to no overlap between positive and negative instances, PMI with only positive training bags can describe the positive instance distribution accurately and also achieves satisfying performance. However, if there exists a big overlap between positive and negative, we will get a poor result though both positive and negative bags are used as the training set. So the result will degrade furthermore with only positive training bags.

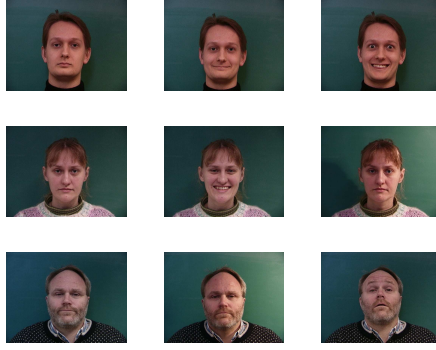


Fig. 4: The face images from three persons in this data set are shown. Each row corresponds one person’s images.

3.2 Face Identification

This experiment shows result of PMI on face identification. The image set [1] is used to evaluate PMI. The task of face identification is predict whether an image contains face(s) or not. Each of these face images contains one person’s face and the similar green background. This image set collects 37 persons’ faces from various views under different light conditions. Three face samples for each person are recorded. So this face image set includes totally 111 face images. Every person has various expressions. These 37 persons include various types: male and female, young and old. Each image is 640×480 size with JPEG file format. No non-face image is provided in this image set. Figure 4 illustrates some examples of this image set. Much more non-face images than face are needed in previous MIL studies. But no non-face image is provided in this data set.

The feature extraction method in [5] is used in our experiments. Only the brief introduction is provided. Please read [6] for more details. The first is to split each image into 4×4 blocks and compute L, U, V mean values of each block in LUV color space. Secondly, 4-order wavelet transformation is applied to L value on each block to compute mean values of LH, HL, HH bands. Each block is transformed into a 6-dimension (L,U,V,LH,HL,HH) feature vector and scaled into $[0, 1]$. We use the toolkit “JSEG” [8] to segment each image into regions. Each region is represented by the mean feature vector of the blocks in this region. So one region corresponds to an instance. An image is associated with a bag. The average instance number of positive bags is 7.8.

Table 4: The numbers of positive bags used for training in PMI and other MIL algorithms are listed.

algorithm	PMI	mi-SVM	MI-SVM	DD	EM-DD
training bag number	111	211	211	211	211

Table 5: The classification accuracies of both traditional MIL methods and PMI.

algorithm	PMI	mi-SVM	MI-SVM	DD	EM-DD
accuracy	90.4 ± 1.9	89.6 ± 1.3	86.5 ± 1.8	85.2 ± 2.4	97.2 ± 1.6

We select 100 background images(for the balance between positive and negative bags) randomly from [4, 14] as negative bags for testing and training in other traditional MIL methods. These

100 negative images contain rich contents and backgrounds. The average instance number of negative bags is about 19. The feature extraction method is the same as that of the face images. The numbers of training bags in PMI and other MIL algorithms are reported in Table 4. The 5-fold cross validation accuracies of both the traditional MIL algorithms and PMI are reported in Table 5. Each accuracy is the average of 10 runs. PMI achieves close performances to the other MIL algorithms. The accuracy of mi-SVM keeps very close to that of PMI. In contrast, MI-SVM and DD fall a little behind the other three methods.

Table 6: The number of queried instances under different ν and γ combinations

$\nu \backslash \gamma$	60	70	80	90	100
0.01	1	1	1	1	1
0.05	1	1	1	1	1
0.1	1	1	1	1	1
0.2	1	1	1	1	1
0.3	1	1	1	1	1
0.5	1	1	1	1	1

To validate Theorem 3, we use all face images as the training set. Table 6 reports the number of queried instances under different parameter combinations of γ and ν . According to Theorem 3, the maximum number of queried instances is larger than $\lceil 7.81 \rceil - 1 = 7$ when $\nu \geq \frac{1}{N} = \frac{1}{111}$. 7.81 is the average instance number of positive bags. The largest number in Table 6 is much smaller than 7, which demonstrates Theorem 3 is correct.

4 Conclusion

This paper proposes a new algorithm PMI, which learns a prediction function with only positive bags. Our proposed algorithm is to reduce the label cost significantly compared with previous MIL algorithms without much accuracy loss. A detailed theoretic analysis is also provided. In most real applications, the queried instance number is much smaller than the theoretical result in Theorem 3 and can be approximated to a constant. The time complexity of PMI is approximated as $O(n^3)$. Experimental results illustrate that PMI usually achieves close performance to those of traditional MIL methods mostly especially when traditional MIL algorithms can predict bag label with a high accuracy. In the future work, we try to apply some dimensional reduction approaches [12, 13, 11] on our proposed method to improve the efficiency.

Acknowledgement

Acknowledge here.

Appendix

Appendix here.

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